NEWS 1 Web Page URLs for STN Seminar Schedule - N. America

NEWS 2 "Ask CAS" for self-help around the clock

NEWS 3 May 12 EXTEND option available in structure searching

NEWS 4 May 12 Polymer links for the POLYLINK command completed in REGISTRY

NEWS 5 May 27 New UPM (Update Code Maximum) field for more efficient patent SDIs in CAplus

NEWS 6 May 27 CAplus super roles and document types searchable in REGISTRY

NEWS 7 Jun 22 STN Patent Forums to be held July 19-22, 2004

NEWS 8 Jun 28 Additional enzyme-catalyzed reactions added to CASREACT

NEWS 9 Jun 28 ANTE, AQUALINE, BIOENG, CIVILENG, ENVIROENG, MECHENG,

and WATER from CSA now available on STN(R)

NEWS 10 Jul 12 BEILSTEIN enhanced with new display and select options, resulting in a closer connection to BABS

NEWS EXPRESS MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT

MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004

NEWS HOURS STN Operating Hours Plus Help Desk Availability

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NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 11:57:19 ON 14 JUL 2004

=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 11:57:28 ON 14 JUL 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 13 JUL 2004 HIGHEST RN 709042-93-3 DICTIONARY FILE UPDATES: 13 JUL 2004 HIGHEST RN 709042-93-3

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

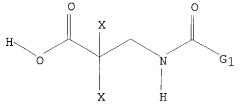
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=>

Uploading C:\Examination Auxillary files\09995987\09995987 third try.str



chain nodes :

1 2 3 4 5 6 7 8 9 10 11 12 14

chain bonds :

 $1-2 \quad 1-12 \quad 2-3 \quad 2-7 \quad 3-4 \quad 3-8 \quad 3-9 \quad 4-5 \quad 5-6 \quad 5-10 \quad 6-11 \quad 6-14$ 

exact/norm bonds : 4-5 5-6 6-11 6-14

exact bonds :

1-12 2-3 3-4 3-8 3-9 5-10

normalized bonds :

1-2 2-7

G1:C,O,S,N

Match level:

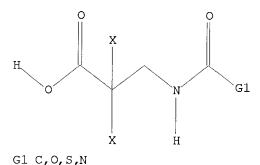
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 14:CLASS

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> search 11 sss sam
SAMPLE SEARCH INITIATED 11:57:56 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 21 TO ITERATE

100.0% PROCESSED

21 ITERATIONS

3 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS:

146 TO 694

PROJECTED ANSWERS:

3 TO 163

3 SEA SSS SAM L1

=> d scan

3 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN L2

D-Valine, N-[N-(5-amino-5-carboxy-1-oxopentyl)-3,3-difluoro-L- $\alpha$ aspartyl]-, (S)- (9CI)

MF C15 H23 F2 N3 O8

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

3 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN L2

3-Furanpropanoic acid,  $\beta$ -[[(1,1-dimethylethoxy)carbonyl]amino]-ΙN

 $\alpha$ ,  $\alpha$ -difluoro- (9CI)

MFC12 H15 F2 N O5

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 3 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

2-Benzofuran<br/>propanoic acid,  $\beta\text{-}[[(1,1\text{-}dimethylethoxy)carbonyl]amino]\text{-}}$ IN  $\alpha, \alpha$ -difluoro- (9CI)

MF C16 H17 F2 N O5

```
O
||
NH-C-OBu-t
|
|
CH-CF<sub>2</sub>-CO<sub>2</sub>H
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\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> search 11 sss full FULL SEARCH INITIATED 11:58:27 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 508 TO ITERATE

100.0% PROCESSED 508 ITERATIONS

22 ANSWERS

SEARCH TIME: 00.00.01

L3 22 SEA SSS FUL L1

=> file c aplus

'C' IS AN AMBIGUOUS FILE OR CLUSTER NAME

CASLINK - Linked CAS files (Predefined Search Sequences)

CASRNS - CAS Registry Numbers Cluster
CHEMENG - Chemical Engineering Cluster
CHEMISTRY - Chemical Literature Cluster
COMPANIES - Files for company based searches

COMPUTER - Computer Science Cluster

CONSTRUCTION - Building and Construction Cluster

CORPSOURCE - Files for STNINDEX corporate source based searches

CURRENT - Current file environment Cluster

CA - The Chemical Abstracts File 1907-present

CABA - CAB ABSTRACTS 1973-present

CANCERLIT - Cancer Literature Online 1963-present
CAOLD - The pre-1967 Chemical Abstracts File

CAPLUS - The Chemical Abstracts Plus File 1907-present
CASREACT - The Chemical Abstracts Reaction Search Service
CBNB - Chemical Business NewsBase from 1984-present

CEABA-VTB - Chem Eng and Biotech Abstr - Verfahrenstechn Ber 1966-

CEN - Chemical & Engineering News 1990-January 2001

CERAB - Ceramic Abstracts from 1976

CFR - Code of Federal Regulations 1997 - present

CHEMCATS - CHEMICAL CATALOGS ONLINE 1993-1997

CHEMINFORMRX - The CHEMINFORMRX Reaction Search Service

CHEMLIST - Regulated Chemicals Listing

CHEMSAFE - chemical safety information

CIN - The Chemical Industry Notes File for 1974-present CIVILENG - Civil Engineering Abstracts 1966 to the present

COMPENDEX - COMPENDEX\*PLUS File from 1970 - present

COMPUAB - Computer & Information Systems Abstracts 1981-present

COMPUSCIENCE - COMPUTERSCIENCE FROM 1972-2002

ENTER FILE OR CLUSTER NAME (IGNORE):end

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

FILE 'CAPLUS' ENTERED AT 11:58:56 ON 14 JUL 2004
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FILE COVERS 1907 - 14 Jul 2004 VOL 141 ISS 3 FILE LAST UPDATED: 13 Jul 2004 (20040713/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 13

L4 14 L3

=> d 14 1-14 ti

- L4 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Preparation of carboxylic acid derivatives that inhibit the binding of integrins to their receptors
- L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Preparation of ureidomethylbenzoylaminodifluoropropionates as glucagon antagonists/inverse agonists.
- L4 ANSWER 3 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Preparation of 3-(N'-oxodihydropyridinylureido)-3-phenylpropanoates as inhibitors of  $\alpha 4\beta 1$  integrin binding
- L4 ANSWER 4 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Synthesis of N,N-disubstituted peptide amides for selectively inhibiting the binding of  $\alpha 4\beta 1$  integrin
- L4 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Preparation of  $\beta$ -amino acid derivatives that inhibit the binding of integrins to their receptors
- L4 ANSWER 6 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Synthesis and evaluation of water-soluble non-prodrug analogs of docetaxel bearing sec-aminoethyl group at the C-10 position
- L4 ANSWER 7 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Synthesis and structure-activity relationships of novel 2',2'-difluoro analogs of docetaxel
- L4 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Preparation of baccatin III derivatives as antitumors
- L4 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Preparation of baccatin III derivatives as antitumors

- L4 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Preparation of taxol derivatives as antitumors
- L4 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Preparation of deacetoxytaxol derivatives as potential antitumors
- L4 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Preparation of taxol derivatives as antitumors
- L4 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Isopenicillin N synthase: a new mode of reactivity
- L4 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Isopenicillin N synthase: a new mode of reactivity

## => d 14 1-5 ti fbib abs

- L4 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Preparation of carboxylic acid derivatives that inhibit the binding of integrins to their receptors
- AN 2004:269913 CAPLUS
- DN 140:287277
- TI Preparation of carboxylic acid derivatives that inhibit the binding of integrins to their receptors
- IN Biediger, Ronald J.; Chen, Qi; Decker, E. Radford; Holland, George W.; Kassir, Jamal M.; Li, Wen; Market, Robert V.; Scott, Ian L.; Wu, Chengde; Li, Jian
- PA USA

to apply the second

- SO U.S. Pat. Appl. Publ., 98 pp., Cont.-in-part of U.S. Ser. No. 707,068. CODEN: USXXCO
- DT Patent
- LA English
- FAN.CNT 3

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US 2001-973142 A 20011009

PATENT FAMILY INFORMATION:

FAN 2000:814302

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PATENT NO. KIND DATE
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    EP 1203766
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                    A2
                           20020508
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    ZA 2001008777
                      Α
                          20030124
                                         ZA 2001-8777 20011024
                                         US 2000-707068 A 20001106
OS
    MARPAT 140:287277
GΙ
```

$$\begin{bmatrix}
Y \\
 & J \\
 & M
\end{bmatrix}$$

$$X \\
 & L$$

$$R4 \quad I$$

AB The invention relates to a method for the inhibition of the binding of α4β1 integrin to its receptors [e.g., VCAM-1 (vascular cell adhesion mol.-1) and fibronectin], compds. that inhibit this binding, and the use of such compds. for the control or prevention of diseases states in which α4β1 is involved. The claims include compds. of general formula I [n is 3-10; Y is CO, N, CR1, CR2R3, NR5, CH, O, S; A is O, S, CR16R17, NR6; E is CH2, O, S, NR7; J is O, S, NR8; T is CO, (CH2)0-3; M is R9R10, (CH2)0-3; L is O, NR11, S, (CH2)0-1; X is CO2B, PO3H2, SO3H, SO2NH2, SO2NHCOR12, OPO3H2, CONHCOR13, CONHSO2R14, OH, tetrazolyl, H; W is C, CR15, N; B, R1-R17 are H, halo, alkyl, alkoxy, acyl, CF3, CO2H, etc.]. Thus, pyridine-containing 3-aminopropionic acid derivative II was prepared by a multistep procedure and showed IC50 = 10 nM in

fibronectin inhibition assay.

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN

TI Preparation of ureidomethylbenzoylaminodifluoropropionates as glucagon antagonists/inverse agonists.

AN 2002:391685 CAPLUS

DN 136:385945

а

TI Preparation of ureidomethylbenzoylaminodifluoropropionates as glucagon antagonists/inverse agonists.

IN Jorgensen, Anker Steen; Madsen, Peter

PA Novo Nordisk A/S, Den.

SO PCT Int. Appl., 85 pp. CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

2111.	PA:	FENT	NO.		KI	ND	DATE			A	PPLI	CATI	ON N	٥.	DATE			
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WO 2001-DK760 W 20011115
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                                           DK 2000-1733
                                                         A 20001117
                                           US 2000-252322PP 20001120
OS
    MARPAT 136:385945
AΒ
     HO2CCF2CH2NHCOZCHR2N(E)XD [R2 = H, alkyl; Z = (substituted) arylene,
     heteroarylene; X = (CH2)q(CR12R13)r(CH2)s, CO(CR12R13)r(CH2)s,
     NR11CO(CR12R13)r(CH2)s, etc.; r = 0, 1; s = 0-3; R11, R12, R13 = H,
     alkyl; D = (substituted) Ph, naphthyl, pyridyl, indenyl, benzothienyl,
     thienyl, furyl, benzofuryl, etc.; E = (substituted) cyclohexyl, Ph, PhCH2,
     PhCH2CH2, indanyl, benzhydryl, etc.], were prepared Thus, Me
     4-[(4-cyclohex-1-enylphenylamino)methyl]benzoate (preparation given) in CH2Cl2
     containing diisopropylethylamine was treated with 3,5-dichlorophenyl
     isocyanate to give a residue which was saponified with LiOH. The resulting
     acid in DMF was treated with 3-[(dimethyliminium)(dimethylamino)methyl]-
     1,2,3-benzotriazol-1-ium-1-olate hexafluorophosphate,
     diisopropylethylamine, Me 3-amino-2,2-difluoropropionate hydrochloride to
     give the uncharacterized amide ester, which was saponified with aqueous LiOH in
     THF/MeOH to give 3-[4-[1-(4-cyclohex-1-enylphenyl)-3-(3,5-
     dichlorophenyl)ureidomethyl]benzoylamino]-2,2-difluoropropionic acid. In
     a human glucagon receptor binding assay, title compds. showed IC50<1000
     nM.
RE.CNT 3
              THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
              ALL CITATIONS AVAILABLE IN THE RE FORMAT
L4
    ANSWER 3 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
ΤI
     Preparation of 3-(N'-oxodihydropyridinylureido)-3-phenylpropanoates as
     inhibitors of \alpha 4\beta 1 integrin binding
ΑN
     2002:349146 CAPLUS
     136:369608
DN
     Preparation of 3-(N'-oxodihydropyridinylureido)-3-phenylpropanoates as
TI
     inhibitors of \alpha 4\beta 1 integrin binding
     Biediger, Ronald J.; Chen, Qi; Holland, George W.; Kassir, Jamal M.; Li,
TN
     Wen; Market, Robert V.; Scott, Ian L.; Wu, Chengde; Decker, Radford E.;
    Li, Jian
PΑ
    Texas Biotechnology Corporation, USA
SO
    Eur. Pat. Appl., 131 pp.
     CODEN: EPXXDW
DT
     Patent
LΑ
    English
FAN.CNT 3
     PATENT NO.
                     KIND DATE
                                          APPLICATION NO. DATE
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                                         EP 2001-125494 20011106
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             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
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DK 2000-1733 A 20001117

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OS
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     Title compds. were prepared Thus, 2-ClC6H4CH2ZNH2 (Z = 4-ethyl-2-oxo-1,2-exp-1)
AΒ
     dihydropyridine-1,3-diyl) (preparation given) was condensed with
     (S)-4-MeC6H4CH(NH2)CH2CO2Et and COC12 to give, after saponification,
     (S)-2-C1C6H4CH2ZNHCONHCH(C6H4Me-4)CH2CO2H (Z as above). Data for biol.
     activity of title compds. were given.
     ANSWER 4 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
L4
     Synthesis of N,N-disubstituted peptide amides for selectively inhibiting
TI
     the binding of \alpha 4\beta 1 integrin
     2001:145268 CAPLUS
AN
DN
     134:193742
TI
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     Biediger, Ronald J.; Grabbe, Vanessa O.; Holland, George W.; Kassir, Jamal
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     M.; Kogan, Timothy P.; Lin, Shuqun; Market, Robert V.; Raju, Bore G.;
     Scott, Ian L.; Wu, Chengde
PΑ
     Texas Biotechnology Corporation, USA
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     U.S., 30 pp., Cont.-in-part of U.S. Ser. No. 292,187.
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OS	MARPAT 134:193742					

GΙ

Peptide amides I [A, J = O, S, or (un) substituted amino; E = CH2, O, S, or AΒ (un) substituted amino; s, t = 0-3; T = CO, bond, CH2, CH2CH2, or CH2CH2CH2; L = O, S, (un) substituted amino, CH2, or CH2CH2; M = bond or (un) substituted alkylene; X = H, CO2H, carboxy ester, PO3H2, SO3H, OPO3H2, C(O)NHC(O)R12, C(O)NHSO2R13, oxazolyl, tetrazolyl, or H; R1-R5, R12, R13 = H, (cyclo)alkyl, aryl, heterocyclyl, etc.] were prepared as selective inhibitors of the binding of  $\alpha 4\beta 1$  integrin to its receptors, such as VCAM-1 (vascular cell adhesion mol.-1) and fibronectin. example, thiophene-2-methylamine was coupled with benzaldehyde and the product used to amidate Boc-L-Lys(Cbz)-OH (Boc = tert-butoxycarbonyl, Cbz = benzyloxycarbonyl). Deprotection and acylation of the  $\alpha$ -amine with (S)-Me 3-[[(p-nitrophenoxy)carbonyl]amino]-3-(1,3-benzodioxol-5yl)propionate and deesterification yielded peptide II. Invention compds. were assayed for their ability to suppress binding using a 26-amino acid peptide containing the CS-1 sequence of fibronectin with N-terminal cysteine coupled to maleimide activated ovalbumin. Sixty of the test compds. inhibited cell adhesion by 99-100% at concns. of 100  $\mu M$  and gave IC50 values ranging from 0.0004 to 40.

RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Preparation of  $\beta\text{-amino}$  acid derivatives that inhibit the binding of integrins to their receptors
- AN 2000:814302 CAPLUS

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DN
     133:362963
     Preparation of \beta-amino acid derivatives that inhibit the binding of
     integrins to their receptors
     Biediger, Ronald J.; Chen, Qi; Holland, George W.; Kassir, Jamal M.; Li,
IN
     Wen; Market, Robert V.; Scott, Ian L.; Wu, Chengde
PΑ
     Texas Biotechnology Corporation, USA
     PCT Int. Appl., 113 pp.
     CODEN: PIXXD2
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$$(Y) q J M X$$

$$W A E T E R4 I$$

Title compds. I [Y, at each occurrence, independently = CO, N, CR1, CR2R3, NR5, CH, O, or S; q = 3-10; A = O, S, CR16R17, NR6; E = CH2, O, S, NR7; J = O, S, NR8; M = CR9R10 or (CH2)0-3; T = CO or (CH2)0-3; L = O, NR11, S, (CH2)0-1; X = CO2B, PO3H2, SO3H, SO2NH2, SO2NHCOR12, OPO3H2, CONHCOR13, CONHSO2R14, tetrazolyl, hydroxyl, H; W = C, CR15, N; B, R1-17 = H, halo, hydroxyl, alkyl, alkoxy, aliphatic acyl, CF3, nitro, cycloalkyl, alkylheteroaryl, sulfonyl, carboxyl, etc.] or their pharmaceutically acceptable salts were prepared for inhibition of the binding of  $\alpha 4\beta 1$  integrin to its receptors. Thus, II was prepared and assayed (IC50 = 0.2  $\mu$ M) for its ability to suppress binding using a

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GΙ

26-amino acid peptide containing the CS-1 sequence of fibronectin with N-terminal cysteine coupled to maleimide activated ovalbumin. THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 3 ALL CITATIONS AVAILABLE IN THE RE FORMAT

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